Finals

1. A Fokker-Plank equation describes the diffusion of a particle in a potential $u(x)$, with

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} + \frac{1}{\xi}\frac{\partial}{\partial x}\left(n\frac{\partial u}{\partial x}\right)$$

For $u(x) = -fx$, with reflecting B.C's at $x = \pm L/2$, analytically determine the steady state solution for $n_\infty(x)$. Numerically integrate the Fokker-Plank equation using any method you choose (for any nonzero ξ and f you choose), and show that your predicted steady state solution is recovered as $t \to \infty$

Answer

For a steady state case, $\partial n/\partial t = 0$

If $u = -fx$, $\frac{\partial u}{\partial x} = -f$

Substituting both results:

$$D\frac{\partial^2 n}{\partial x^2} + \frac{1}{\xi}\frac{\partial}{\partial x}(n \cdot -f) = 0$$

$$D\frac{\partial^2 n}{\partial x^2} - \frac{f}{\xi}\frac{\partial n}{\partial x} = 0$$

Let $\partial n/\partial x = n'$, the PDE becomes

$$D\frac{\partial n'}{\partial x} = f/\xi \, n'$$

$$\frac{D\xi}{f}\frac{\partial n'}{n'} = \partial x$$

Integrating b/s between $L/2$ and $-L/2$

$$\frac{D\xi}{f}\int\frac{\partial n'}{n'} = \int \partial x$$

$$\frac{D\xi}{f}\ln n' = x + c \qquad c \to \text{const.}$$

$$\ln n' = \frac{f}{D\xi}(x+c)$$

$$n' = e^{\frac{f}{D\xi}(x+c)}$$

$$\frac{\partial n}{\partial x} = e^{f/D\xi \, x} \cdot e^{c} =$$

$$\int \partial n = k \cdot \int e^{\frac{f}{D\xi}x}\,dx = k \cdot \frac{D\xi}{f}e^{\frac{f}{D\xi}x} + C_2 \quad \left[\text{where } k = e^{c}\right.$$

$$n = k \cdot \frac{D\zeta}{f} e^{\frac{f}{D\zeta}x} + C_2$$

Numerical simulation : FTCS

Using the simplified F-P :

$$D \frac{\partial^2 n}{\partial x^2} - \frac{f}{\zeta} \frac{\partial n}{\partial x} = \frac{\partial n}{\partial t}$$

Discretize using FTCS

$$D \frac{n_{i+1}^t - 2n_i^t + n_{i-1}^t}{(\Delta x)^2} - \frac{f}{\zeta} \frac{n_{i+1}^t - n_{i-1}^t}{2\Delta x} = \frac{n_i^{t+1} - n_i^t}{\Delta t}$$

$$\frac{D}{(\Delta x)^2} n_{i+1}^t - \frac{2D}{(\Delta x)^2} n_i^t + \frac{D}{(\Delta x)^2} n_{i-1}^t - \frac{f}{2\zeta\Delta x} n_{i+1}^t + \frac{f}{2\zeta \Delta x} n_{i-1}^t - \frac{n_i^{t+1}}{\Delta t} + \frac{n_i^t}{\Delta t} = 0$$

$$\left(\frac{D}{(\Delta x)^2} - \frac{f}{2\zeta\Delta x}\right) n_{i+1}^t - \left(\frac{2D}{\Delta x^2} - \frac{1}{\Delta t}\right) n_i^t + \left(\frac{D}{(\Delta x)^2} + \frac{f}{2\zeta\Delta x}\right) n_{i-1}^t = \frac{n_i^{t+1}}{\Delta t}$$

$$n_i^{t+1} = \Delta t \left[\left(\frac{D}{\Delta x^2} + \frac{f}{2\zeta\Delta x}\right) n_{i-1}^t - \left(\frac{2D}{\Delta x^2} - \frac{1}{\Delta t}\right) n_i^t + \left(\frac{D}{\Delta x^2} - \frac{f}{2\zeta\Delta x}\right) n_{i+1}^t\right]$$

$$n_i^{t+1} = n_i^t + D\frac{\Delta t}{\Delta x^2}\left[\left(1 + \frac{f \cdot \Delta x}{2\zeta D}\right) n_{i-1}^t - 2n_i^t + \left(1 - \frac{f\Delta x}{2\zeta D}\right) n_{i+1}^t\right]$$

How The Reflecting B.C is implemented

$$\left.\frac{\partial n}{\partial x}\right|_{\pm L/2} = 0$$

at 1st grid ($-L/2$): $\frac{n_{i+1} - n_{i-1}}{\Delta x} = 0$ $\qquad n_0 = n_2$

$$n_1^{t+1} = n_1^t + D\frac{\Delta t}{\Delta x^2}\left[-2n_1^t + 2n_2^t\right]$$

at last grid ($L/2$) : $\quad n_{N+1} = n_{N-1}$

$$n_N^{t+1} = n_N^t + D\frac{\Delta t}{\Delta x^2}\left[2n_{N-1}^t - 2n_N^t\right]$$

2. Numerically solve for the wavefunction of a particle approaching a δ function potential, satisfying

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + u\delta(x)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

with the natural units $\hbar = m = 1$, using a Crank-Nicholson scheme. Use the periodic B.C $\psi(-L/2) = \psi(L/2)$ for $L = 1000$ (in dim-less units), and take the initial condition to be a traveling Gaussian packet $\psi(x,0) \propto e^{ipx/\hbar - \frac{(x-x_0)^2}{2\sigma^2}}$ representing a particle moving towards the δ function barrier with momentum p. You should use $x_0 = -L/4$, $p = 1$, and $\sigma = 20$ (all in dim-less units). Show that for $u = 0.5$ and $u = 2.0$, the wave packet is partially transmitted and partially reflected. Numerically compute the amplitude of the transmitted and reflected packets for $u = 0.5$ and 2.0.

Solution

The 'schro' code by Garcia was for a free particle. I modified it to include u. Since u was multiplied by a delta function, I added it to the hamiltonian, at a chosen location $\rightarrow N/5$

Also, since momentum, $p = mv$

$$\frac{ipx}{\hbar} = ix.\left(\frac{mv}{\hbar}\right)$$

where $k_0 = mv/\hbar$